

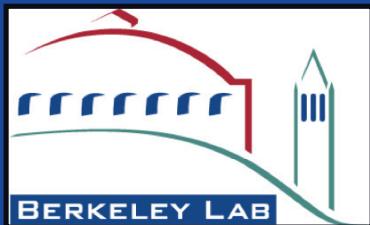
# Integrated Hydrogeophysical and Hydrogeologic Driven Parameter Upscaling for Dual-Domain Transport Modeling



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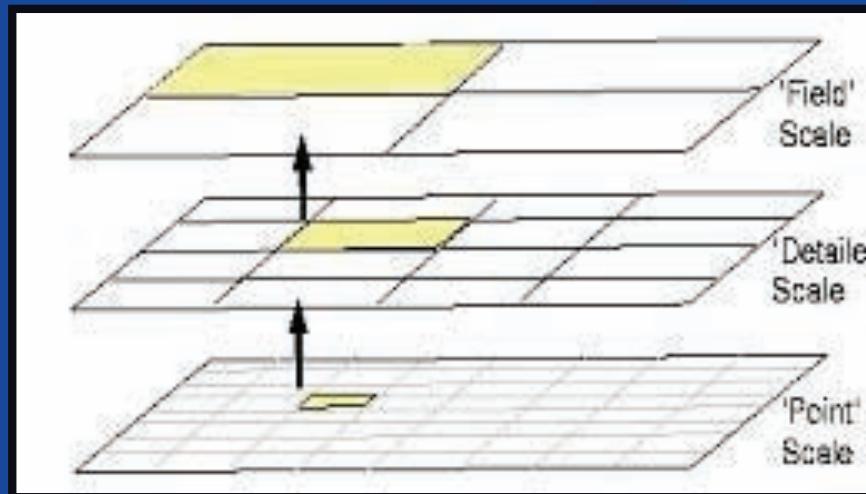
Grant No. DE-FG02-06ER64210



April 9, 2008

# Research Motivation

1. “...field observations to determine spatially distributed model parameters have been sparse and inadequate due to limitations in the ability to characterize large domains of heterogeneous subsurface materials and the mismatch in small-scale observations and their representation at larger modeling scales.” U.S. Dept. of Energy
2. Conventional modeling approaches that rely on these sparse data sets typically do not successfully predict long-term plume behavior with sufficient accuracy to guide remediation strategies.



# Research Hypothesis

Improved prediction of contaminant transport can be achieved using a dual-domain transport approach driven by integration of hydrogeophysical and hydrogeological parameter estimation and upscaling



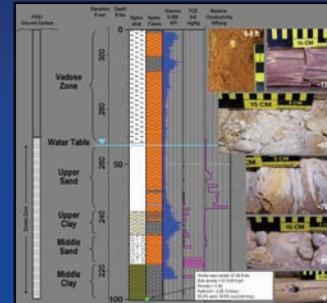
# Research Objectives

1. Develop dual-domain modeling approach that relies on field-measurable attributes (incorporate the primary interactions between mobile and immobile transport regions that play an important role in long-term plume behavior)
2. Develop facies-based multi-scale field characterization approach incorporating geophysical logs, crosshole, and surface characterization with hydrogeologic estimation of hydraulic conductivity
3. Evaluate the combined methodologies (i.e., data integration and dual-domain modeling) by applying the process to prediction of plume behavior at SRS P-Area

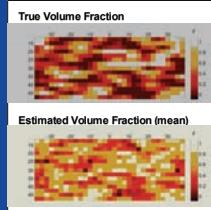
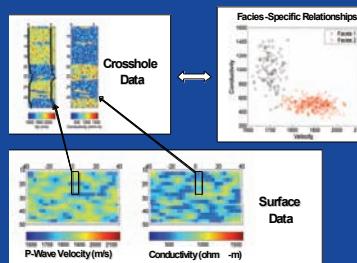


# Research Components

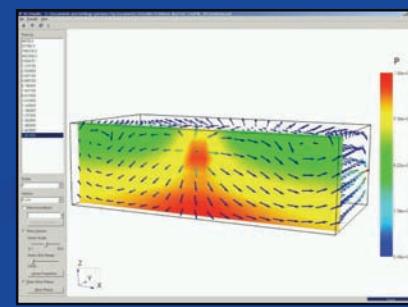
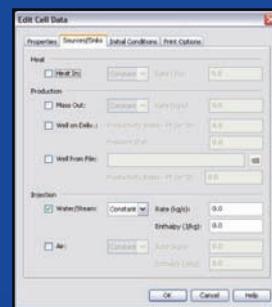
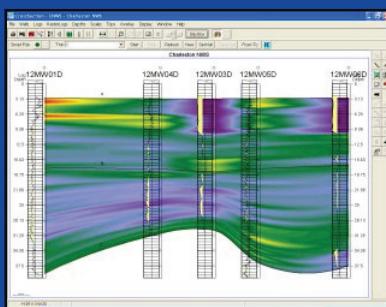
- Multi-parameter, multi-scale field investigations



- Stochastic data integration and parameter upscaling



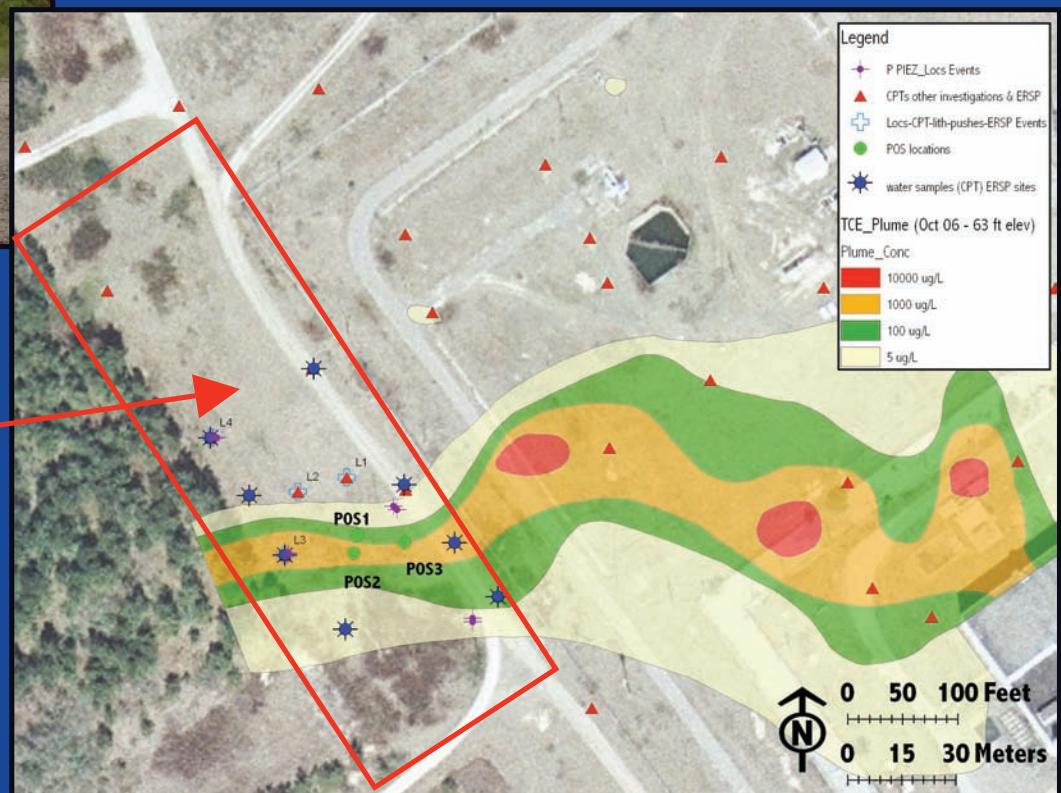
- Dual-domain transport modeling



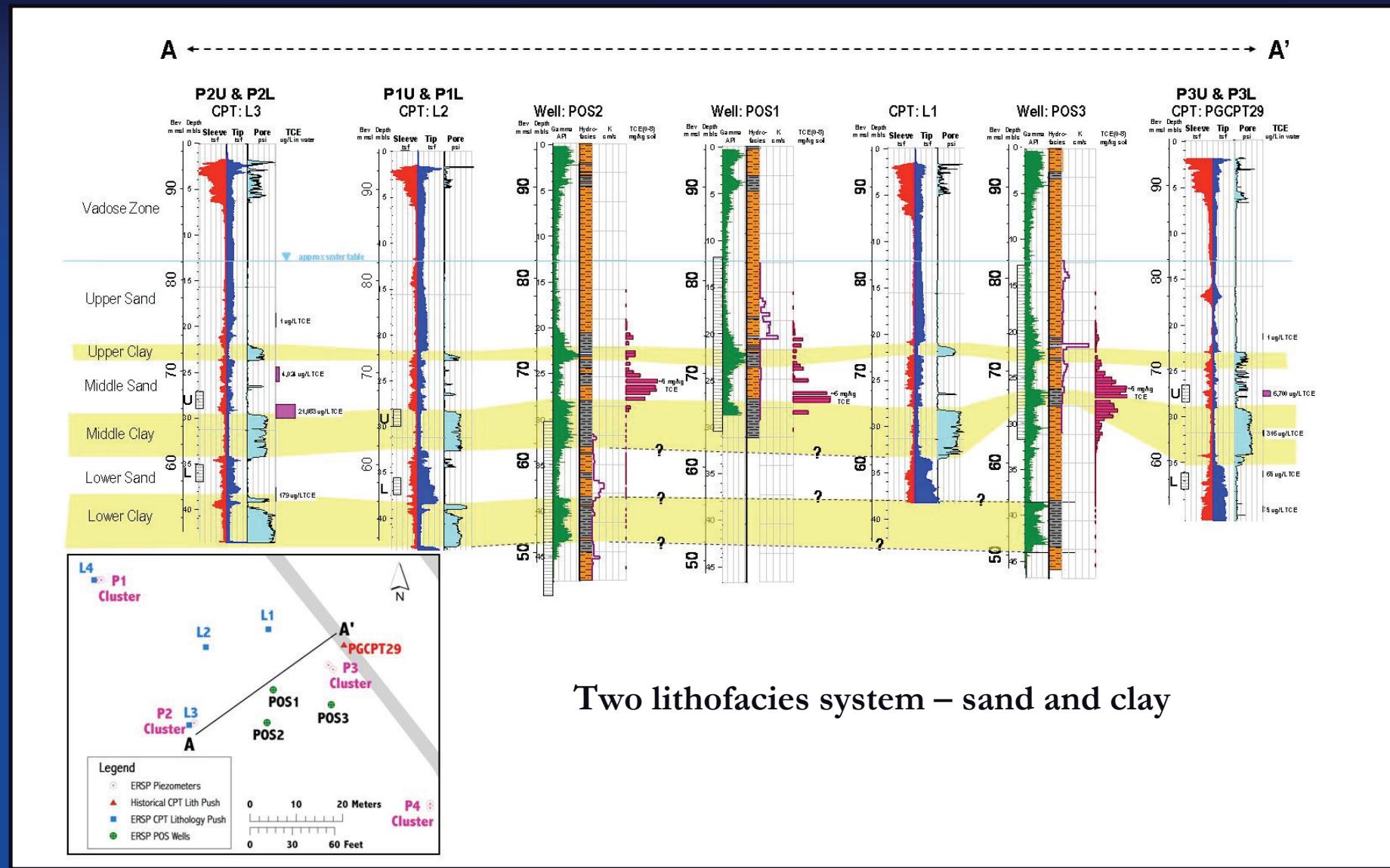
# Study Site - SRS P-Area



Several plumes have been identified at this site; the plume of interest is a trichloroethylene (TCE) plume that emanates from the northwest section of the reactor facility and discharges to nearby Steel Creek

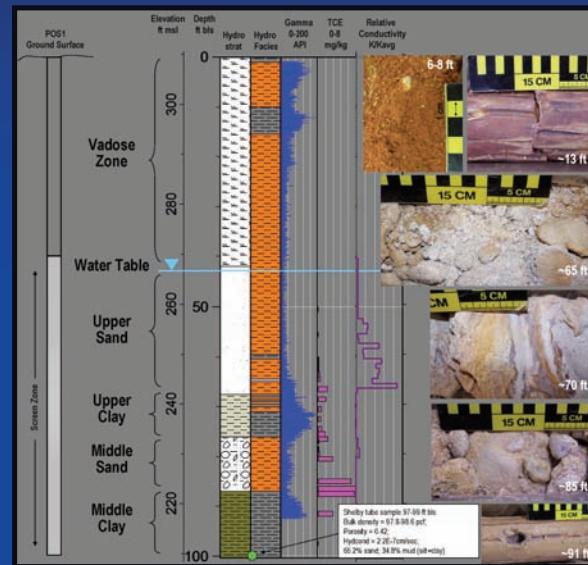
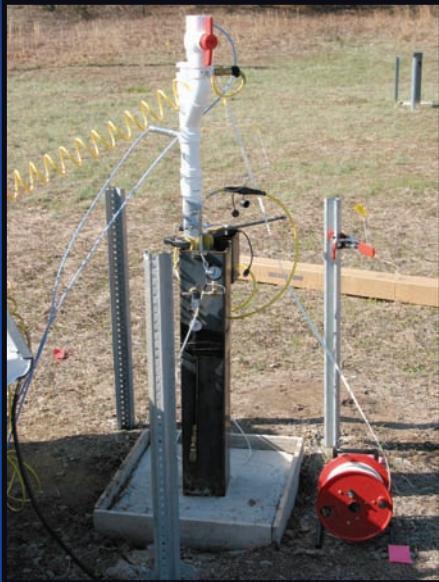


# Subsurface Characteristics of Study Site

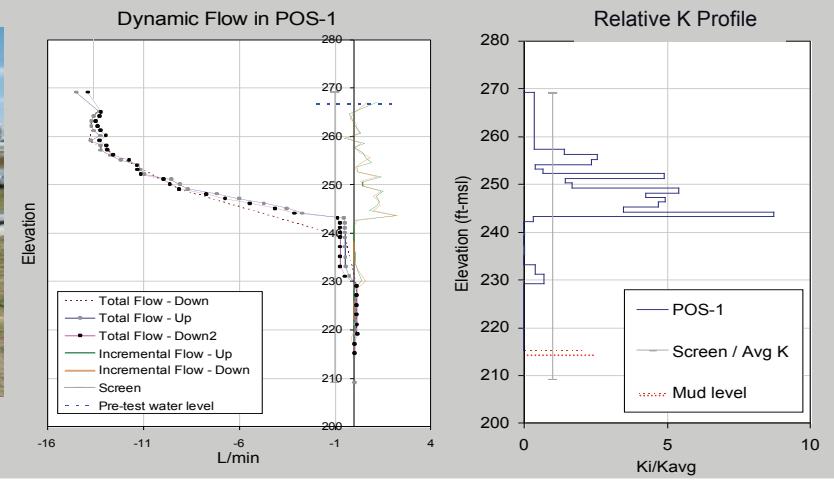


# Field/Subsurface Data Types and Spatial Scales

Small-Scale Borehole Data – e.g., core data, geophysical logs, and flowmeter data

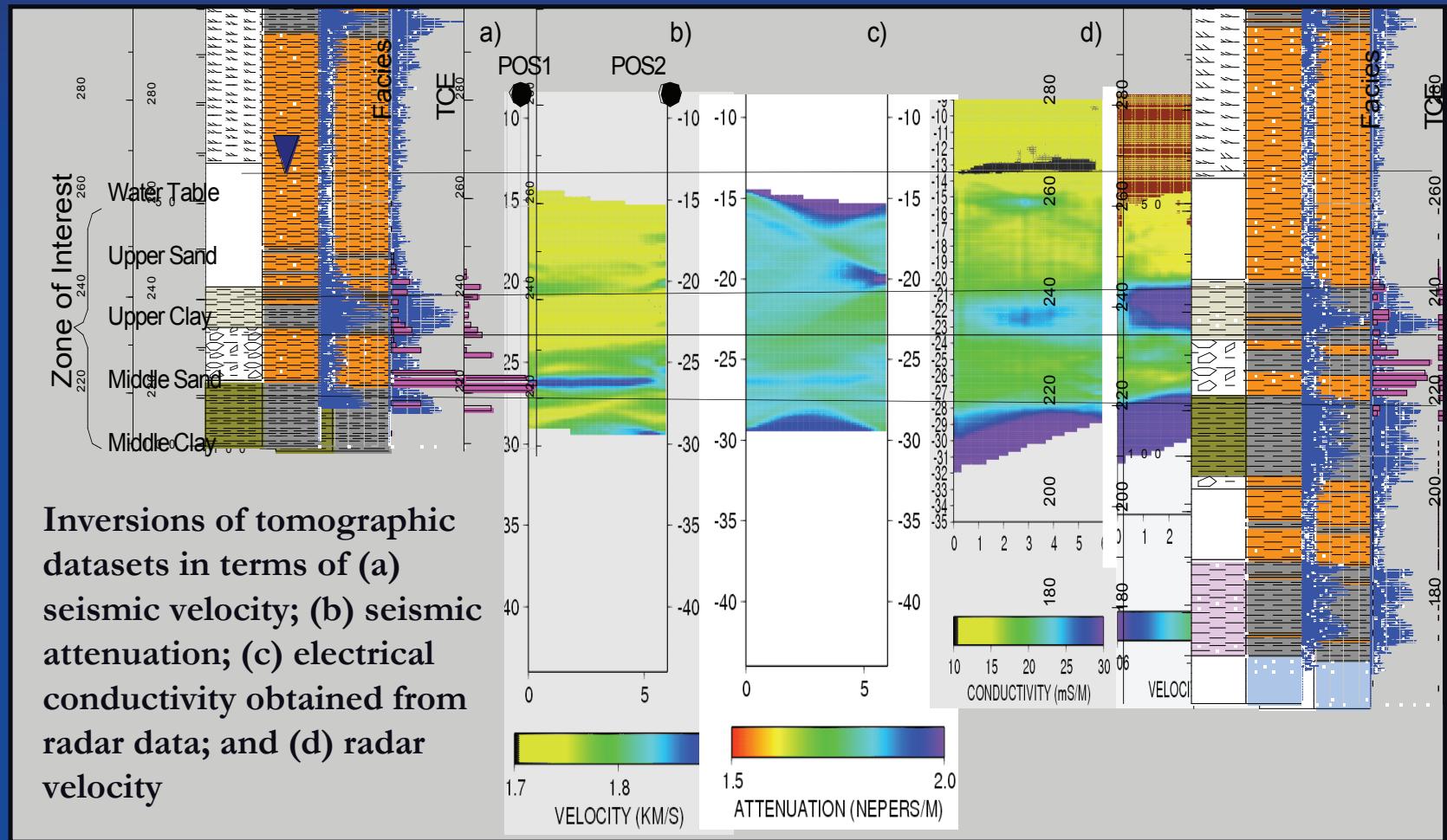


- Bulk properties
- Permeability
- Particle size
- Dry sieve analyses
- Core description



# Field/Subsurface Data Types and Spatial Scales

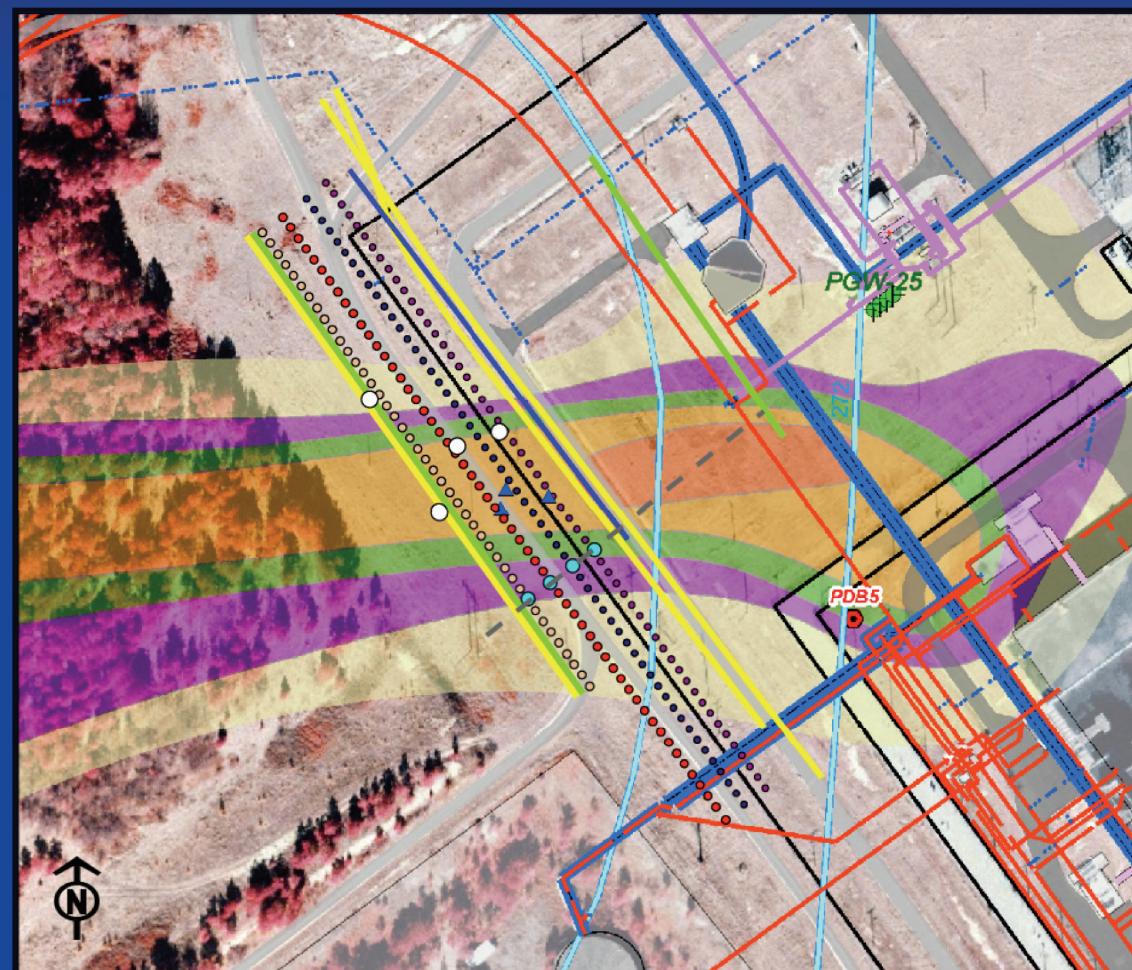
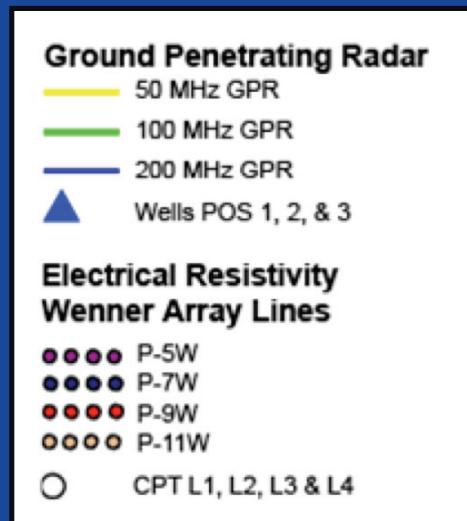
Intermediate-Scale Crosshole Data – e.g., tomographic radar, seismic, and electrical resistivity data



# Field/Subsurface Data Types and Spatial Scales

**Large-Scale Surface-Based Data – e.g., GPR, electrical resistivity, and seismic data**

Locations of GPR  
and ERT Surveys

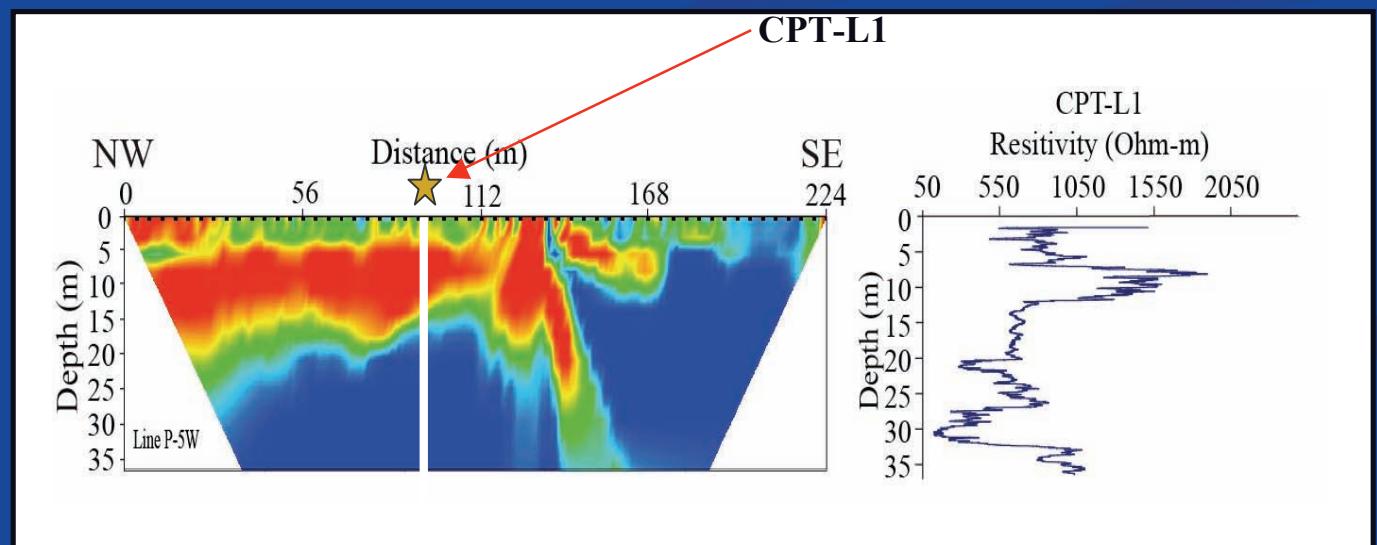


# GPR and ERT Data Sets



100 MHz GPR reflection section

ERT profile  
using the  
Wenner array



# Pseudo 3D Surface Seismic Reflection Survey

- Survey area = 34 m X 170 m
- 2906 shot points
- Group spacing = 1 m
- Line spacing = 2 m
- Sample rate = 0.5 ms
- Record length = 500 ms
- Target depth = 35 m

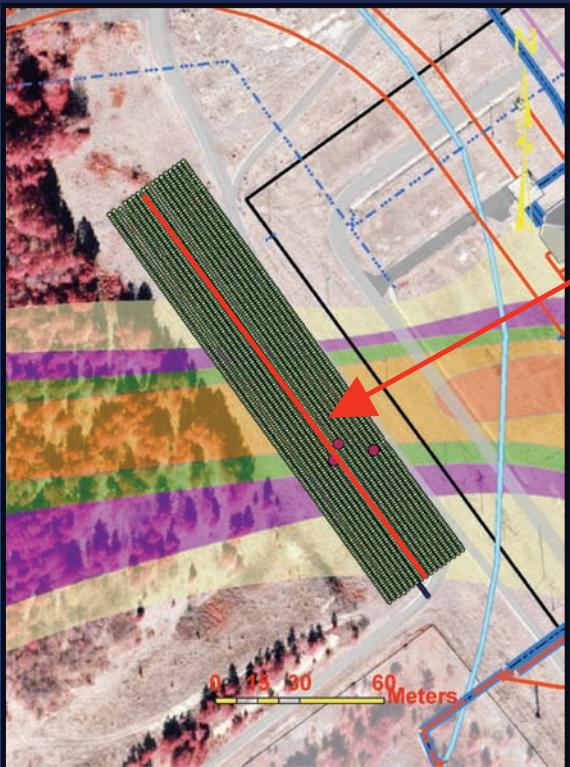
Accelerated hydraulic weight drop system used for seismic source, flags are locations of receivers



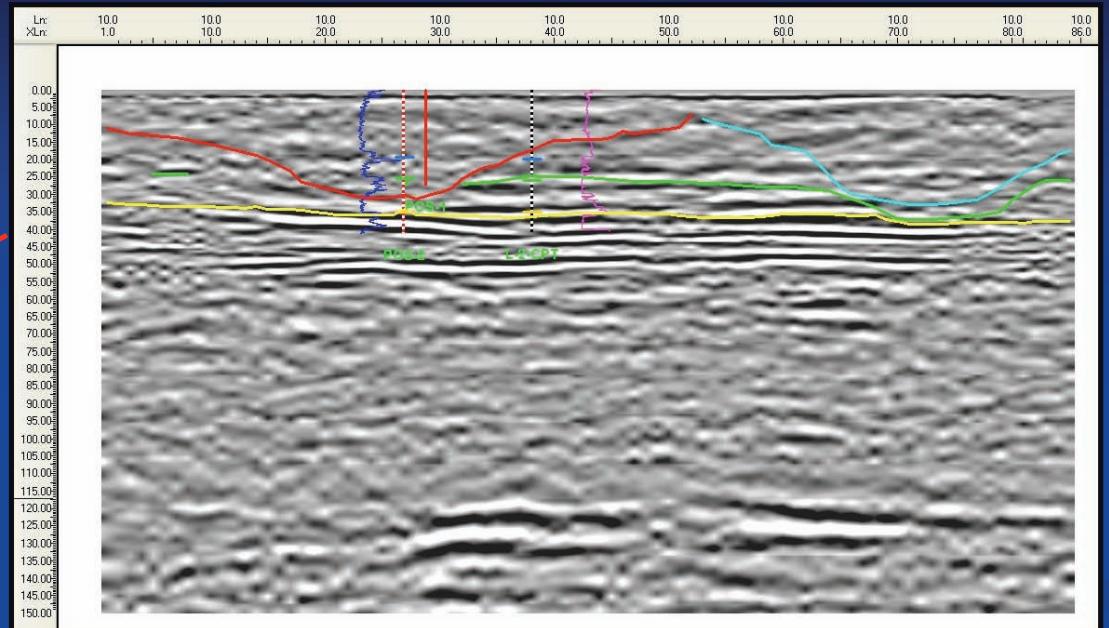
- Resulting data processed as 3D cube
- Provides 3D perspective on conceptual site model developed from borehole data



# Pseudo 3D Surface Seismic Reflection Survey



Map view of seismic survey layout – 17 inlines and 86 crosslines

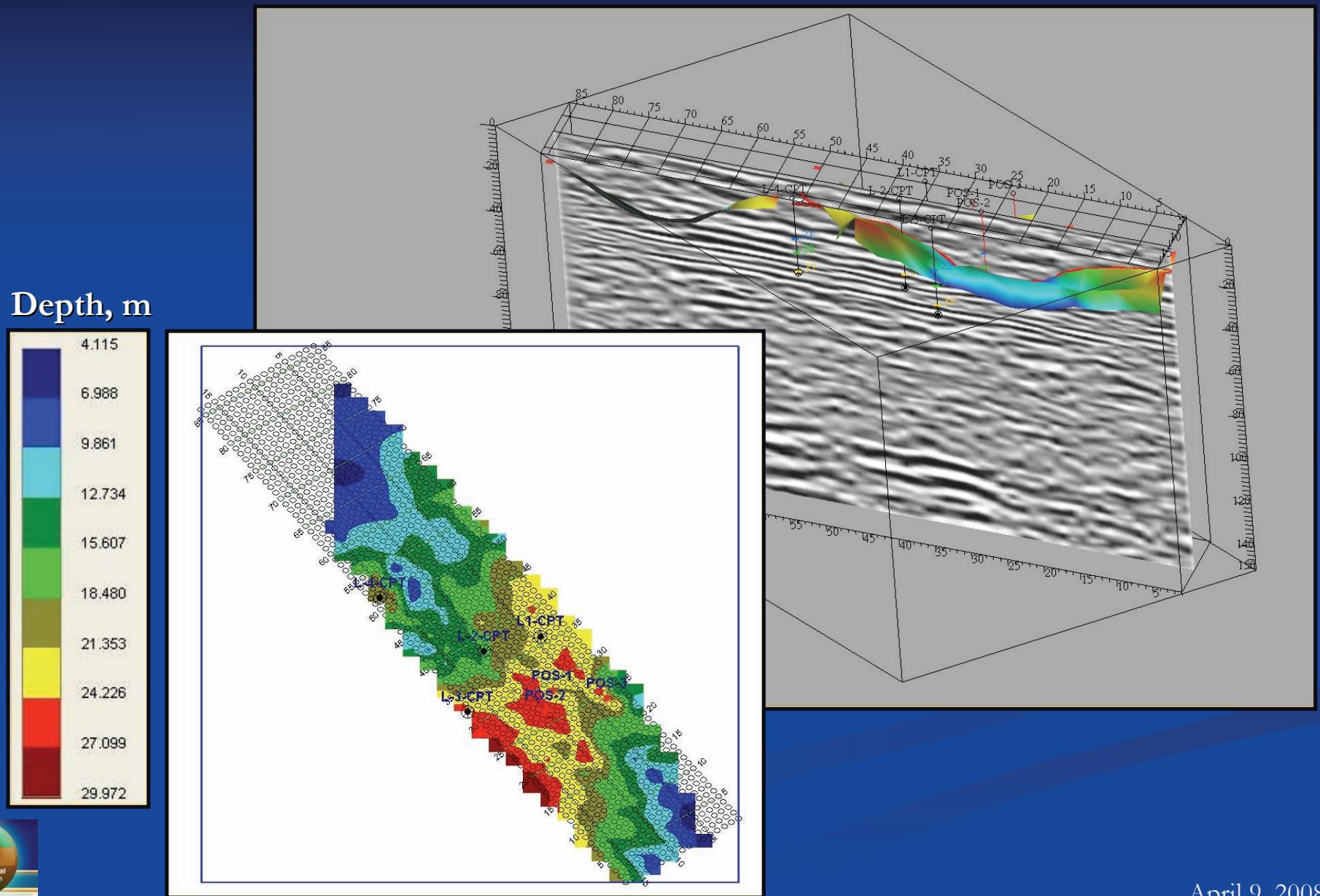


Blue horizon = top of upper clay  
Green horizon = top of middle clay  
Yellow horizon = top of lower clay  
Cyan = channel feature  
Red = channel feature

Shows two prominent channel features; one has incised down through the upper and middle clays; one has cut into sand unit below the lower clay

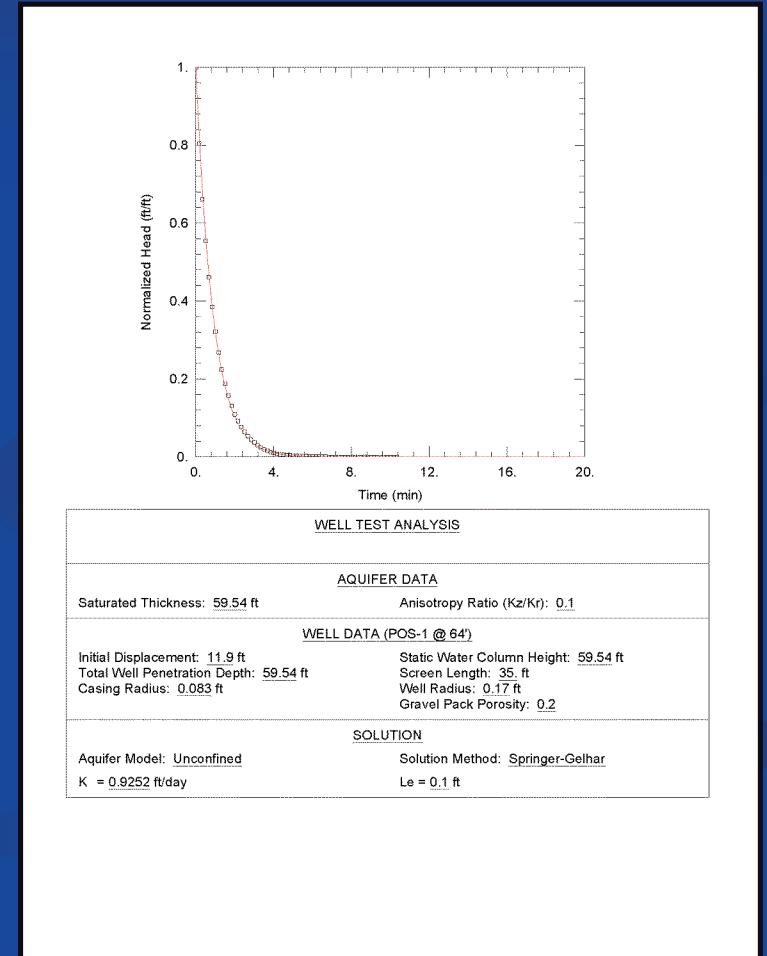
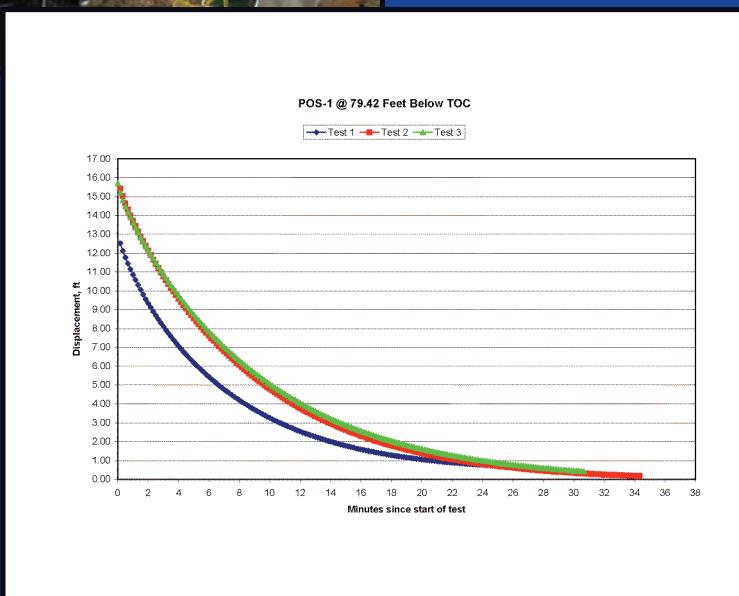


# Pseudo 3D Surface Seismic Reflection Survey



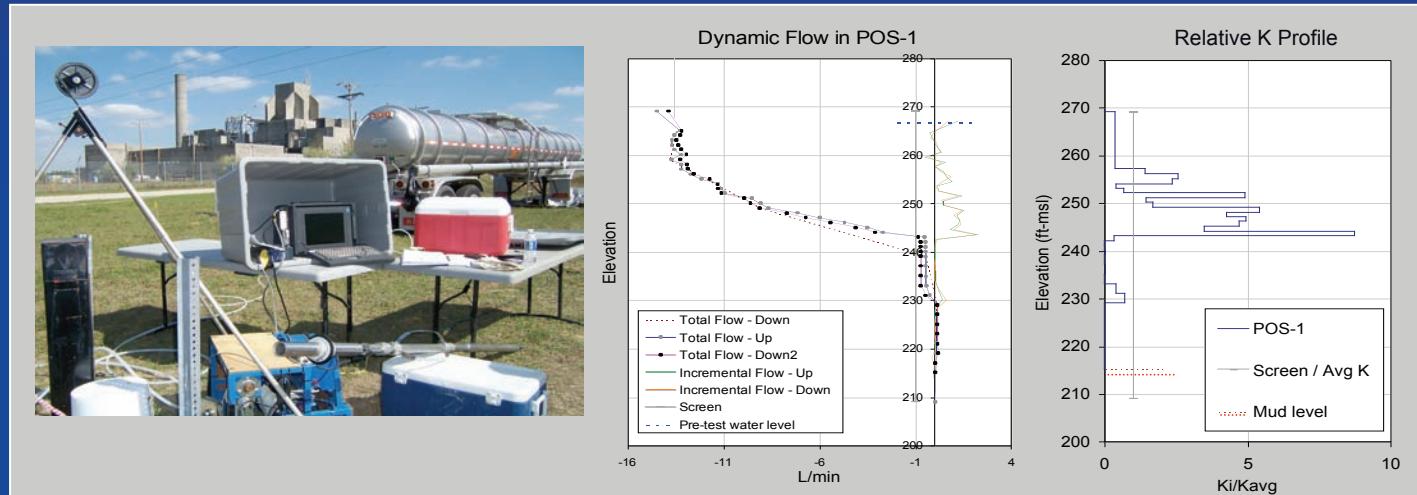
# Hydrogeologic / Hydrologic Data (Multiple Scales)

- Single borehole conductivity (i.e., slug) tests (small-scale)



# Hydrogeologic / Hydrologic Data (Multiple Scales)

- Electromagnetic borehole flowmeter tests (small-scale)



- Falling head permeability tests (small-scale)
- Multi-well aquifer pumping tests (intermediate-scale)

# **Summary of Characterization Findings**

- + Six sand and clay layers of interest below the water table
- + Bulk of TCE appears to be located in the Middle Sand (TCE also occurs below Middle Clay in some areas)
- + Surface seismic indicates discontinuities in upper and middle clay units within the study area
- + Crosshole tomography between POS wells shows intermediate-scale variations in lithology
- +/- Preliminary hydraulic conductivity estimates are revealing but suspect due to well completion issues
- Spatial extent of crosshole data is limited
- Surface GPR is attenuated by clays
- Groundwater level data are “interesting” but measuring point elevations need to be confirmed



# **Field Investigations Ongoing Work**

- Another round of characterization wells and piezometers to be installed
- Additional crosshole work
- Slug testing piezometers and new characterization wells
- Firm up potentiometric surface data with well survey
- Multi-well aquifer pumping test
- Additional flowmeter tests

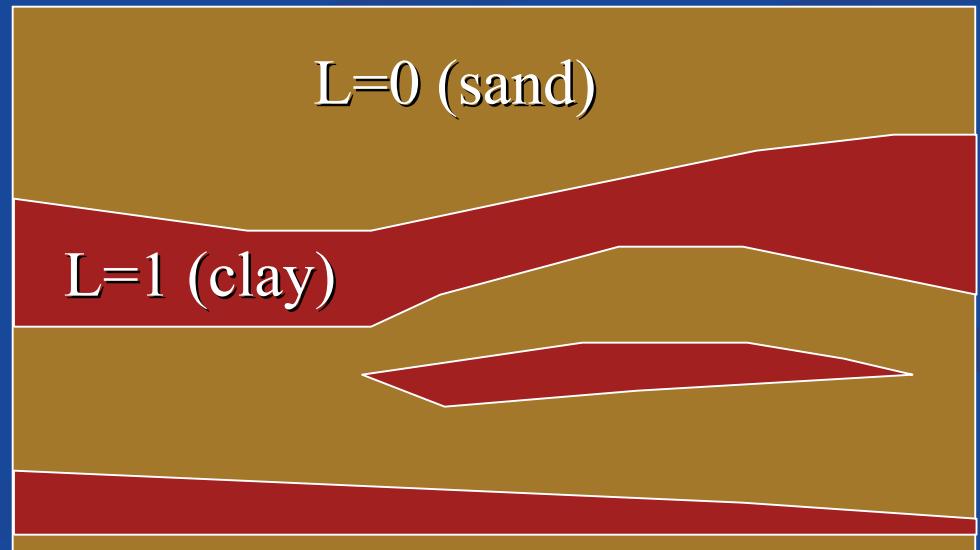


# Multi-Scale Data Integration Framework

## Description:

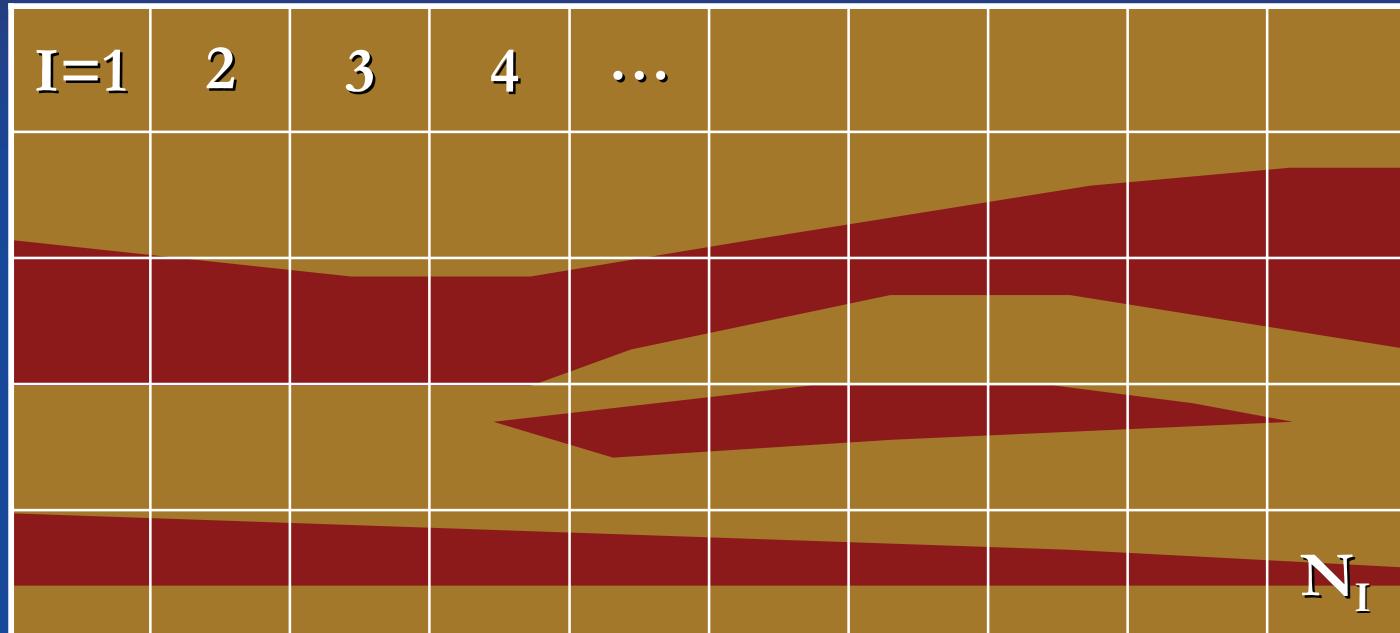
- Methodology to integrate various hydrogeophysical data types that span a wide range of spatial scales (i.e., point, local, subregional)
- Incorporate large-scale surface geophysical data, intermediate scale cross-hole geophysical data, and small scale borehole/petrophysical data into field-scale transport model
- Stochastic (Bayesian) methodology
- Lithofacies-based approach
- “Dual-domain” example

## Conceptual Model



# Multi-Scale Data Integration Framework

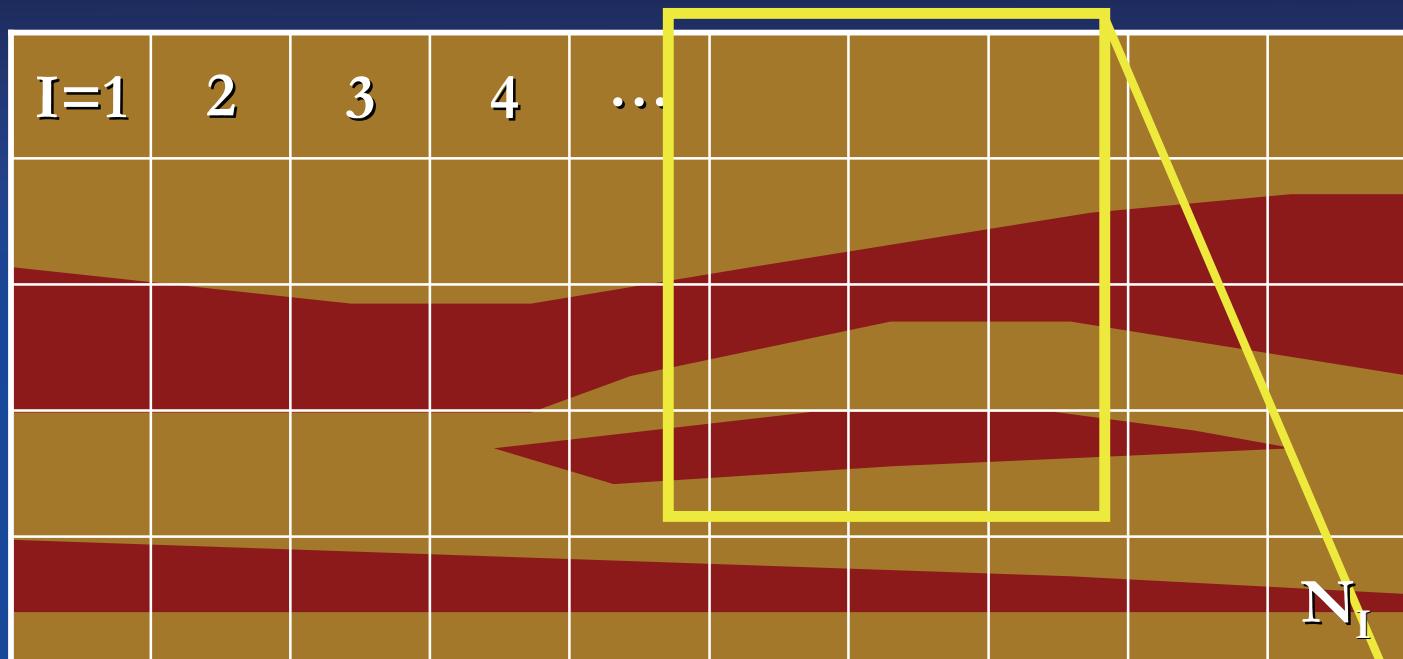
## Large-Scale Site Characterization Data



Surface geophysics (e.g., seismic and resistivity)  $V_I$  and  $R_I$



# Multi-Scale Data Integration Framework



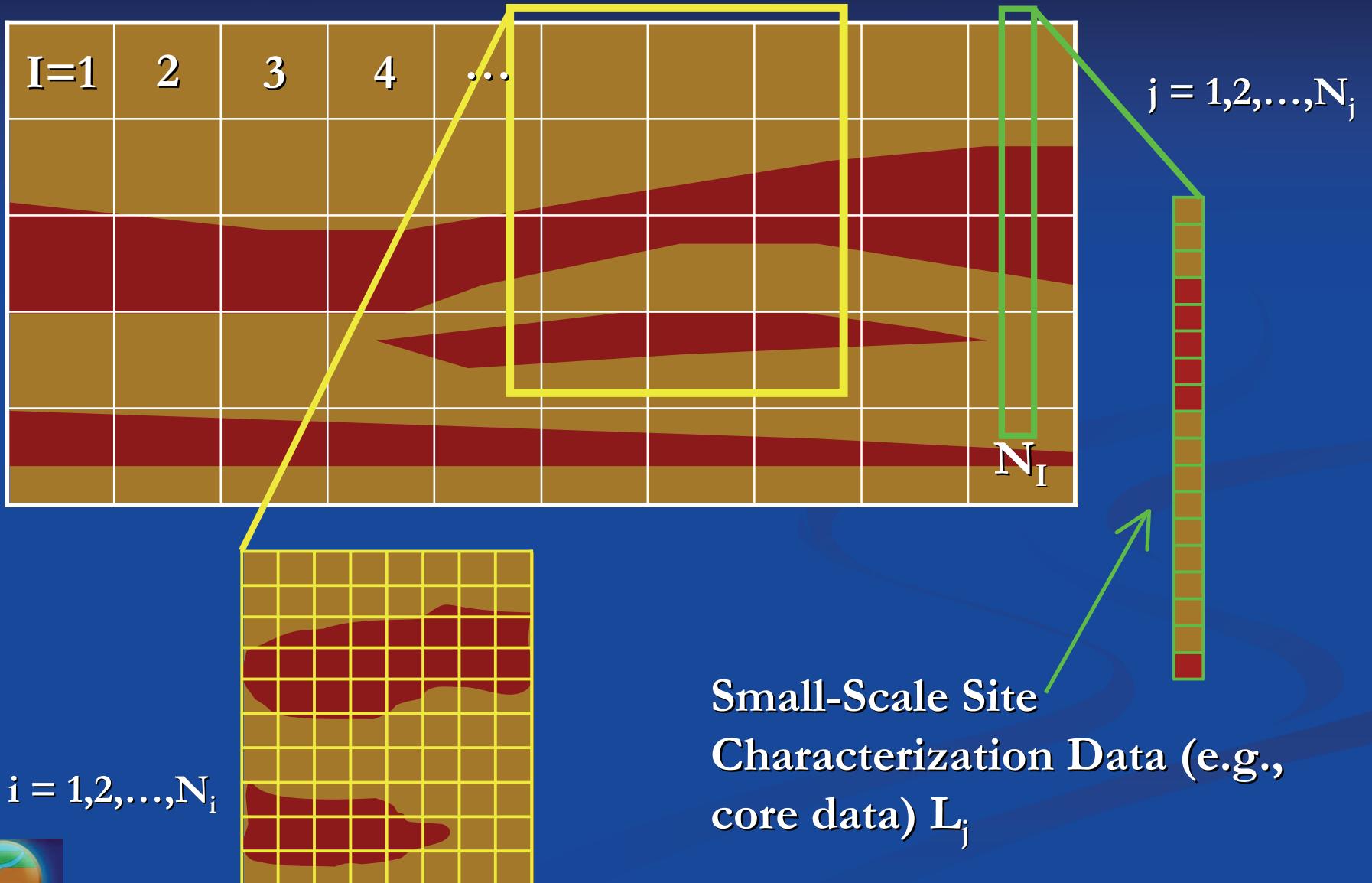
Intermediate-Scale Site  
Characterization Data (e.g.,  
crosshole seismic and  
resistivity)  $V_i$  and  $R_i$



$i = 1, 2, \dots, N_i$

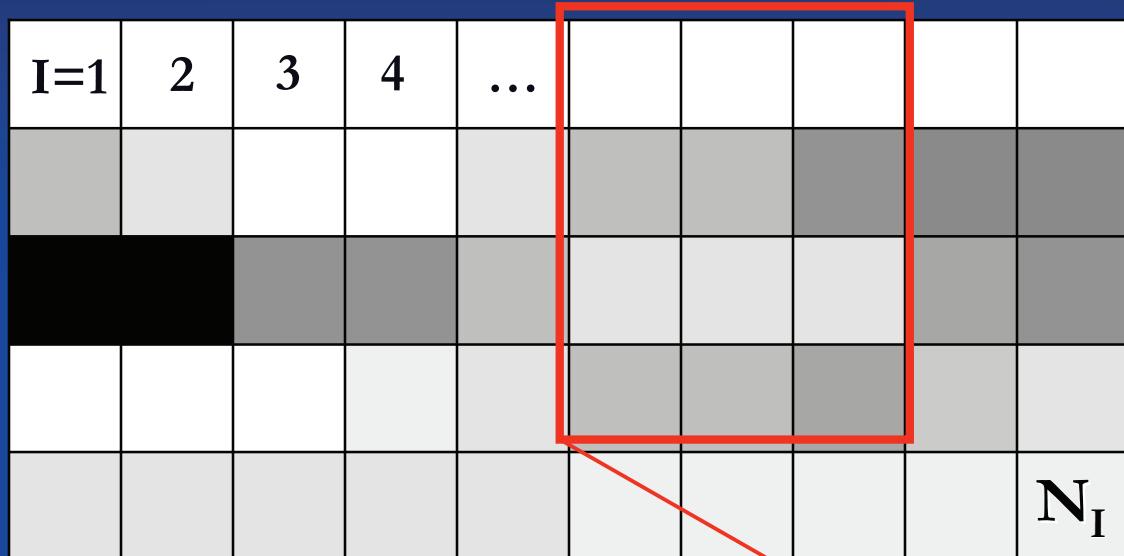


# Multi-Scale Data Integration Framework

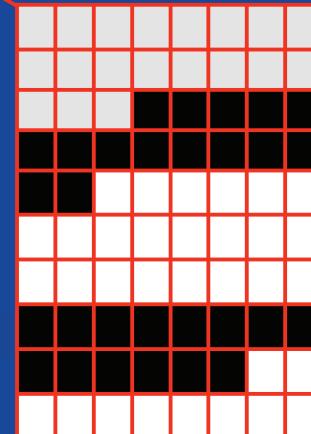


# Multi-Scale Data Integration Framework

Unknowns =  $F_I$  and  $L_i$



$F_I$  : Lithofacies volume fraction (between 0 and 1) at each large-scale pixel  $I$



$L_i$  : Lithofacies type (0 or 1) at each small-scale pixel  $i$   
 $i = 1, 2, \dots, N_I$

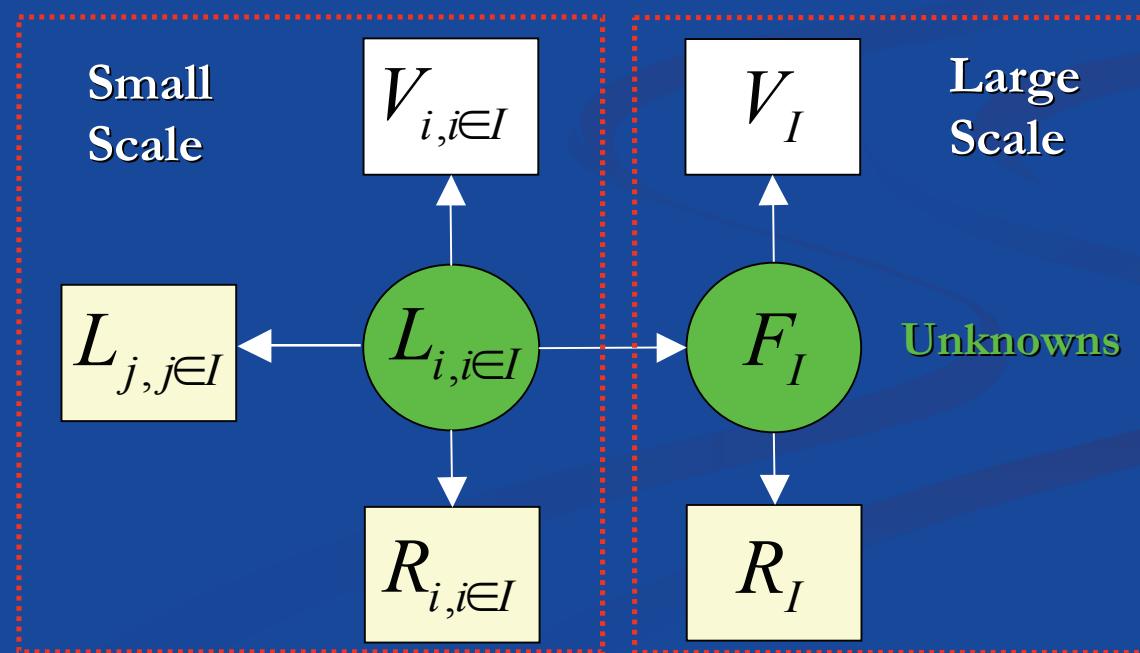
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# Multi-Scale Data Integration Framework

## Bayesian Approach to Estimating the Spatial Distribution of $F_I$ and $L_i$

- Conditioned to borehole and surface data
- Unknown variables  $F_I$  and  $L_i$  are considered random variables
- Unknown variables  $F_I$  and  $L_i$  are characterized by joint conditional probability density functions (pdfs)

Model of  
Dependence  
Among  
Parameters  
and Data



# Multi-Scale Data Integration Framework

## Procedure:

### 1. Derive conditional distributions

$$[V_I, R_I | F_I]$$

$$[F_I | L_{i,i \in I}]$$

$$[L_{i,i \notin I} | V_{i,i \notin I}, R_{i,i \notin I}, L_{j,j \neq i}]$$

### 2. MCMC sampling method (Chen et al., 2004)

- Efficiently draw samples to obtain marginal pdfs
- Monitor convergence

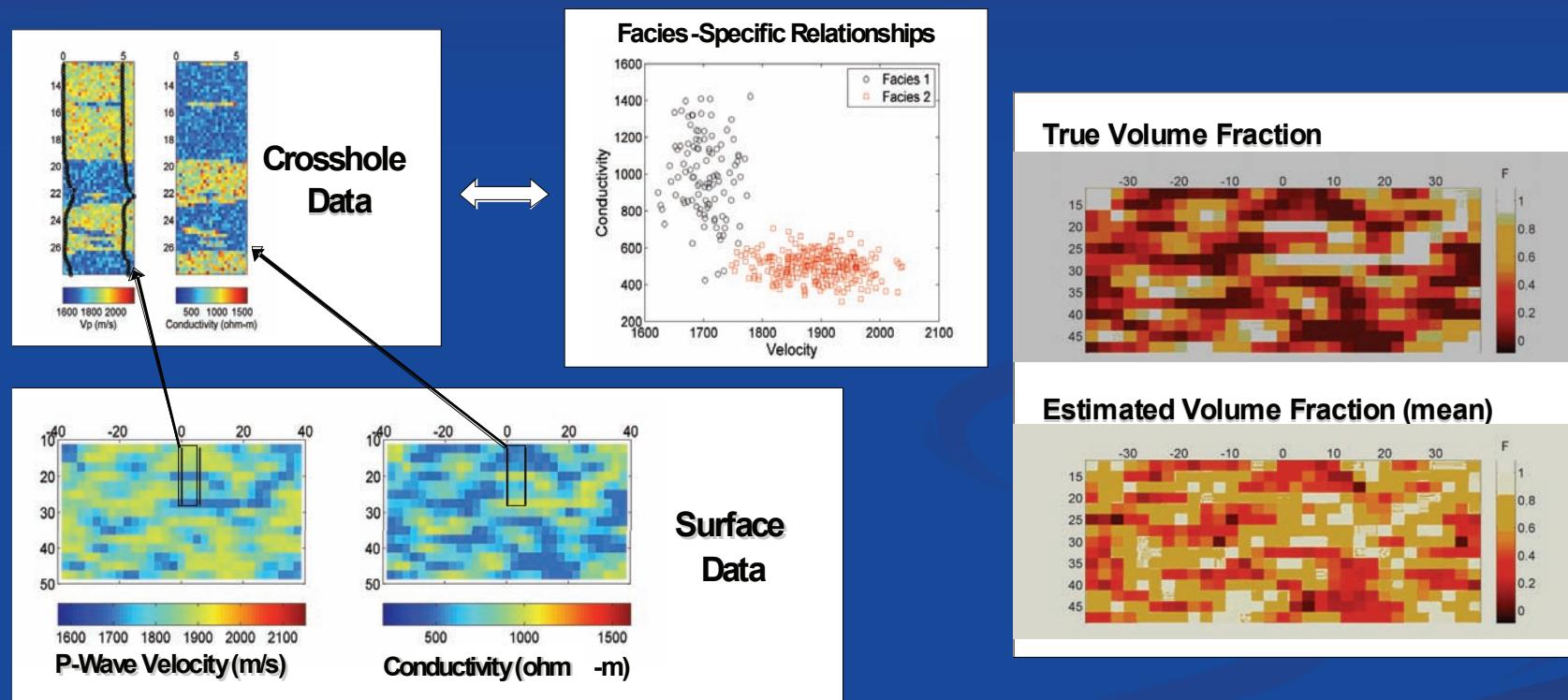
### 3. Infer unknown parameter distributions at each pixel

$$[F_I, L_{i,i \in I} | V_I, R_I, V_{i,i \in I}, R_{i,i \in I}, L_{j,j \neq i}]$$



# Multi-Scale Data Integration Framework

Test of the Multi-Scale Data Integration Methodology Using Synthetic Data



# Data Integration Ongoing Work

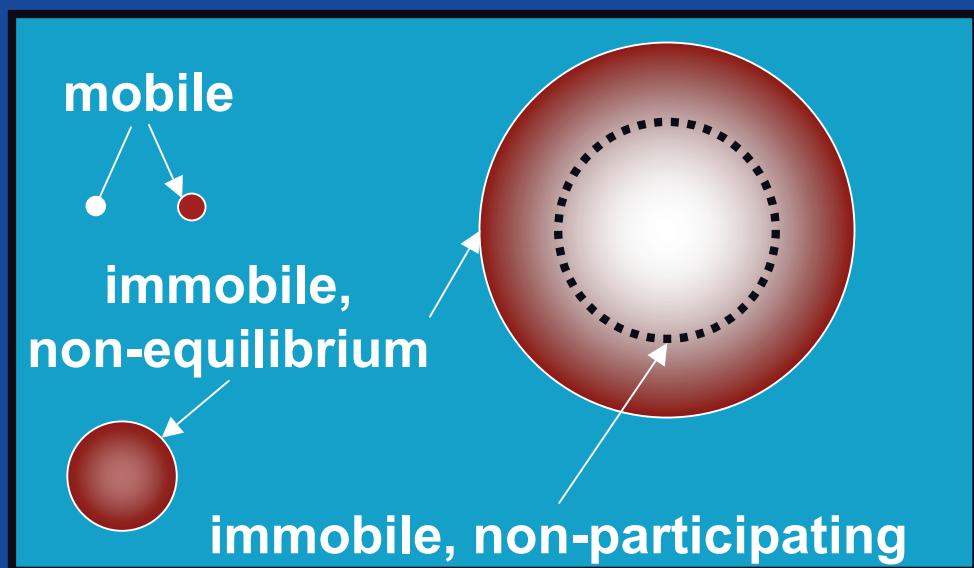
- The statistical model is being developed for site-specific conditions
- The relationships between data types and unknowns are not yet known for our site
- Synthetic models are being developed assuming reasonable relationships
- Final formulation will depend on ultimate needs for the dual-domain model formulation



# Dual-Domain Modeling

## Background:

- Porous continuum divided into two interacting domains – a mobile domain where transport is dominated by advection and an immobile domain where advective transport does not occur – plus a third non-participating domain
- Hydrodynamic dispersion and mass transfer between zones with high hydraulic conductivity contrasts are used to account for heterogeneity at scales smaller than those explicitly represented within the model domain



Note: the presence of immobile water does not imply an immobile, non-equilibrium classification



# Non-Dimensional Formulation (no sorption)

Four parameter system ( $\beta_{im}$   $\beta_{np}$   $Pe_\theta$   $Da_\theta$ ) given  $U$   $L$   $\theta$ :

$$\frac{\partial C_m}{\partial t'} + \beta_{im} \frac{\partial C_{im}}{\partial t'} = \frac{1}{Pe_\theta} \frac{\partial^2 C_m}{\partial x'^2} - [1 + \beta_{im} + \beta_{np}] \frac{\partial C_m}{\partial x'} \quad \text{whole domain}$$

$$\frac{\partial C_{im}}{\partial t'} = Da_\theta [C_m - C_{im}] \quad \text{immobile domain (mass transfer)}$$

Dimensional parameters:

$$\theta_m = \frac{\theta}{1 + \beta_{im} + \beta_{np}} \quad \theta_{im} = \beta_{im} \theta_m \quad \theta_{np} = \beta_{np} \theta_m \quad \text{porosities}$$

$$D = \frac{UL}{\theta Pe_\theta} \quad \begin{matrix} \text{diffusion} \\ \text{coefficient} \end{matrix}$$

$$\zeta = \frac{Da_\theta U}{L} \frac{\beta_{im}}{1 + \beta_{im} + \beta_{np}} \quad \begin{matrix} \text{mass transfer} \\ \text{coefficient} \end{matrix}$$



# Dual-Domain Model Hypotheses

Dual-domain parameters are a function of:

- Permeability field
- Flow field
- Mass transfer time scales
- Time scale of contaminant exposure  
(and thus not a property of the porous medium)

Optimal parameter settings can be reasonably related to field measurable site attributes:

- Effective conductivity given flow orientation  
(e.g., flow model calibration, aquifer test)
- Summary statistics of K distribution (e.g., harmonic mean)
- Correlation length scale of low K features (geologic characterization)
- Contaminant exposure time

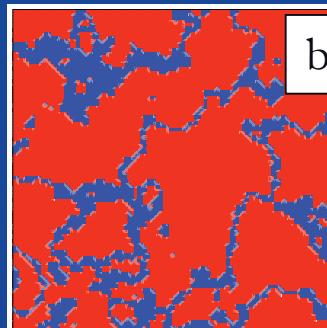
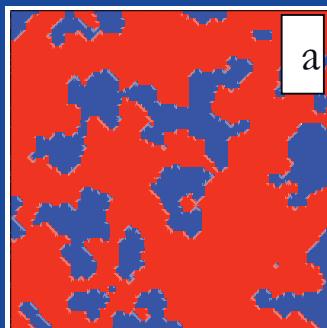


# Dual-Domain Numerical Experimentation

2700 non-dimensional 2D simulations to date

Attributes varied:

- Discrete versus continuous K distribution
- Facies proportion and K contrast (discrete)
- Variance (continuous)
- Connectedness of high K (suppressed, neutral, enhanced)
- Anisotropy
- Flow orientation with respect to anisotropy
- Low K spatial correlation length
- Peclet number (effective diffusion coefficient)
- Contaminant exposure (injection) time



Example: Connectivity  
of high-K (blue) facies  
at 25% proportion: a)  
neutral, b) enhanced



# Dual-Domain Modeling Selected Findings

Low immobile and non-participating porosity when:

- Low K contrast (discrete) or variance (continuous)
- Small-scale spatial correlation
- Low connectivity of high K (flow cannot bypass low K)
- Flow perpendicular to strata (flow cannot bypass low K)

Mass transfer time scale primarily related to the mean solute residence time ( $t_0$ ), and mildly to contaminant exposure time or experiment duration

- $Da_\theta$  close to, but less than, 1

Dispersion follows conventional rule of thumb (dispersivity = 10% of travel length) using mobile domain velocity

- $Pe = 10$



# Dual-Domain Modeling Ongoing Work

Quantitatively relate optimal dual-domain parameter settings to practical system measures:

- Preliminary correlations are promising, but
- Additional interpretation is needed

Validate dual-domain modeling methodology at SRS P-Area field site:

- Use geophysical information to select optimum parameters
- Compare dual-domain transport to TCE plume



# Results Dissemination

- Cameron A. E., C. Knapp, A. Addison, and M.G. Waddell, (2007), Delineation of Shallow Hydrostratigraphy using Ground Penetrating Radar and Electrical Resistivity Methods at the P Reactor Area, Savannah River Site, South Carolina, *Geological Society of America Southeastern Section Annual Conference, Abstract with Programs*, Vol. 39, No. 2.
- Cameron, A., C. Knapp, A. Addison, M.G. Waddell, (2006), Applications of Ground Penetrating Radar for hydrogeologic characterization at the P Reactor Area, Savannah River Site, South Carolina, *Eos Trans. AGU, 87(52)*, Fall Mtg., Suppl., Abstract H31B-1411.
- Flach, G.P, et al., (2008), (Title to be determined – Topic: Dual-domain Numerical Experimentation Using Synthetic Heterogeneity), *Water Resources Research* (in preparation).
- Kowalsky, M., S. Hubbard, J. Chen, J. Peterson and G.P. Flach, (2007), Multiscale Hydrogeophysical Data Integration for Parameterization of Transport Model at Savannah River Site, *Eos Trans. AGU, 88(52)*, Fall Mtg. Suppl., Abstract H14C-01 INVITED.
- Waddell, M.G., A. Addison, D. Brantley, and J.M. Shafer (2008), Using Pseudo 3D P-wave Seismic Reflection Data in Developing a More Robust Geologic Conceptual Model in Site Characterization: An Example from P-Area, Savannah River Site, SC, *AAPG Annual Mtg. (Abstract)*, San Antonio, TX, April 2008.



# The End



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